3-Hydroxy-4-methoxy-benzaldehyde 621-59-0 | DTXSID7049423

6	21-59-0	DTXSID7049423	

Model Performance

_			
N	Model	Data	

Weighted KNN model

5-fold CV (5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.84	0.55	0.85	0.53	0.83	0.64	

Model Results

Predicted value: 2.62

Global applicability domain: Inside

Local applicability domain index: 5.33e-01

Confidence level: 7.45e-01

Nearest Neighbors from the Training Set

Image not found

Paraldehyde Measured: 3.02 Predicted: 2.77

Image not found

2-Isopropyl-6-methyl-4pyrimidone Measured: 1.82 Predicted: 2.23

Image not found

2,2-Bis(bromomethyl)-1,3-propanediol

Measured: 4.79 Predicted: 3.35

Image not found

2,2-Dimethylpropane-1,3-diol

Measured: 4.68 Predicted: 4.44

Image not found

2,2,4-Trimethyl-1,3-pentanediol

Measured: 1.00 Predicted: 1.47